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Numerical approximations to the treatment of interface roughness scattering in resonant tunnelling diodes

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Abstract. Current calculations for a resonant tunnelling diode which include a self-consistent Born treatment of interface roughness combined with full charge self-consistency are presented. Approximate but more computationally tractable solutions which either ignore the scattering-assisted charge or the real part of the self-energy are compared with the full solution. The coherent tunnelling calculation combined with quantum charge self-consistency provides an accurate estimate of the resonant current. To obtain the same accuracy while including interface roughness scattering for our particular device requires a treatment of both the real and the imaginary parts of the self-energy combined with a fully self-consistent treatment of the scattering-assisted charge.

1. Introduction

Electron transport through a resonant tunnelling diode (RTD) is a function of the electron charging, bandstructure, and scattering effects. The relative importance of these physical effects depends on the device design, device composition and the temperature. To model these effects for layered heterostructures, we developed a comprehensive device simulator [1–7] called NEMO (nanoelectronic modelling), which addresses the design and analysis needs of device engineers and physicists. The underlying theory is documented in detail in [5].

In this paper, we use NEMO to study numerical approximations to the treatment of incoherent elastic scattering resulting from interface roughness (IR) with varying average island sizes of $\Lambda = 0, 5, 10, 40, 100$ nm. An increasing IR average island size implies an increasing strength of the scattering self-energies for small transverse momenta [5, 6]. An exponential correlation model is used [5, 6]. Incoherent averaging is appropriate when the dephasing length exceeds the average island size. The 100 nm island size is pushing the validity of this approach and we are using it to test the numerical convergence properties of our algorithms. Scattering is treated with self-energies calculated in the self-consistent Born approximation using the non-equilibrium Green's function formalism. The self-energies have two effects: they both shift and broaden the resonance spectrum in the RTD and they inject electrons into unoccupied states. Combined, both effects change the electron density in the well of the RTD, which in turn modifies the electrostatic and exchange-correlation [8] potentials. A charge self-consistent treatment is required if the scattering is strong enough. Previously, we presented a finite-order treatment of IR and polar-optical phonon scattering with a fully self-consistent treatment of the charge [2]. Here we present the first self-consistent Born treatment of IR scattering with a fully self-consistent treatment of the charge. We refer to simulations which include scattering-assisted charge in the potential as 'fully charge self-consistent'.

A fully self-consistent treatment is numerically expensive since the scattering must be calculated multiple times in the iterative potential scheme. To reduce this computational load, we can calculate the potential without scattering and then perform a single-pass scattering calculation using the no-scattering-based potential. We refer to such a model as 'partially charge self-consistent'.

Other approaches [9, 10] have modelled scattering with an optical potential of the type $i\hbar/2\tau$ on the diagonal of the Hamiltonian characterized by a relaxation time τ. The physical picture to keep in mind here is that of a damped oscillator. Friction in this oscillator is not only going to widen the resonance spectrum ($\mathrm{Im}\,(\Sigma^R) \approx \hbar/2\tau$) but also shift the centre frequency ($\mathrm{Re}\,(\Sigma^R)$). Ignoring the real part of the self-energy is a numerically appealing since it reduces the shift in the resonance and therefore increases the rate of convergence of the self-consistent Born calculation. In this paper we examine the effects of $\mathrm{Re}\,(\Sigma^R)$ on the I–V characteristic of an RTD with both partial and full charge self-consistency.

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We find that the fully charge self-consistent treatment, including the altered resonance spectrum and scattering-assisted charge, closely reproduces the resonant current calculated from a coherent tunnelling model. Since the full calculation requires approximately 2000 times the CPU time of the coherent tunnelling calculation, it is tempting to use approximations such as partial charge self-consistency or to ignore the real part of the self-energy. However, such approximations can lead to spurious shapes of the resonant current.

2. Partial charge self-consistent simulations

The simulated device is a nominally symmetric GaAs/AlAs RTD consisting of 3.1 nm barriers and a 6.2 nm well. The RTD is clad with 20 nm undoped spacers and highly doped (1×10^{18} cm^{-3}) contact layers. The first and the third heterostructure interfaces are assigned to have IR [6] (see the inset of figure 1(*a*)). All simulations are performed at 4.2 K to avoid Γ–X–Γ tunnelling in the AlAs barriers.

First, we compare the inclusion and exclusion of the real part of the scattering self-energies for partial charge self-consistent simulations. If the real part of the scattering self-energy is included (see figure 1(*a*)), the I–V peak becomes more distorted for increasing scattering strengths. Such distortions of the main I–V peak have been observed by other authors as well [11, 12]. We will show in section 3 that these distortions disappear when a full charge self-consistent calculation is performed.

One numerical approximation applied in earlier work [7, 9, 10, 13] is the neglect of the real part of the self-energies. This approximation improves numerical convergence since the resonances do not move as strongly in energy. For a single polar optical phonon scattering event with partial self-consistency, this approximation actually improves the agreement between simulations and experiment [7] by removing a large distortion of the peak simular to the one shown in figure 1. For a self-consistent Born treatment of IR, neglect of the real part of the self-energy always degrades the results. Figure 1(*b*) shows that the distortion of the shape of the current peak is altered and the peak amplitude is reduced if the real part of the scattering self-energy is excluded from the simulation. The distortion of the peak shape is shown for a single IR correlation length of $\Lambda = 40$ nm in figure 2 in comparison with experimental data.

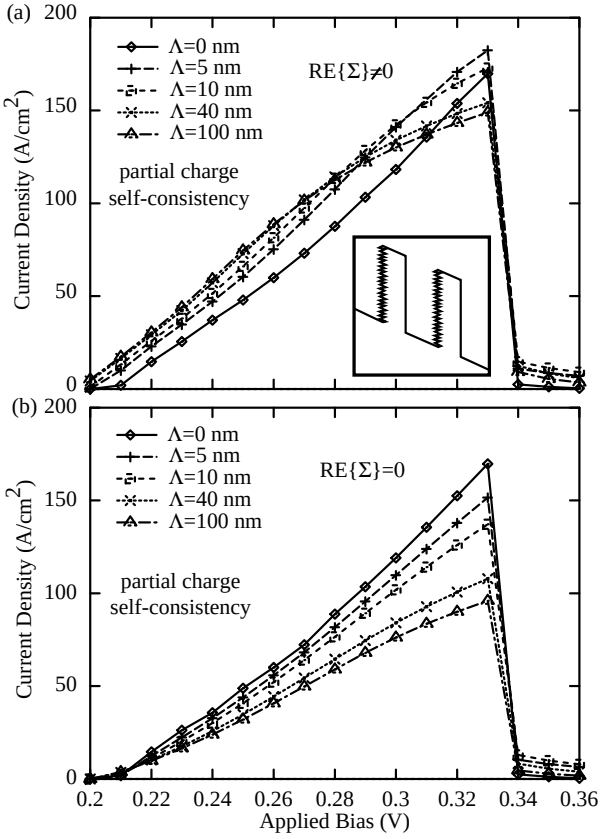

Figure 1. I–V characteristic for four different IR correlation lengths (Λ) computed on a partial charge self-consistent potential (*a*) including and (*b*) excluding the real part of the scattering self-energies. The inset shows the conduction band edge under bias indicating the rough interfaces.

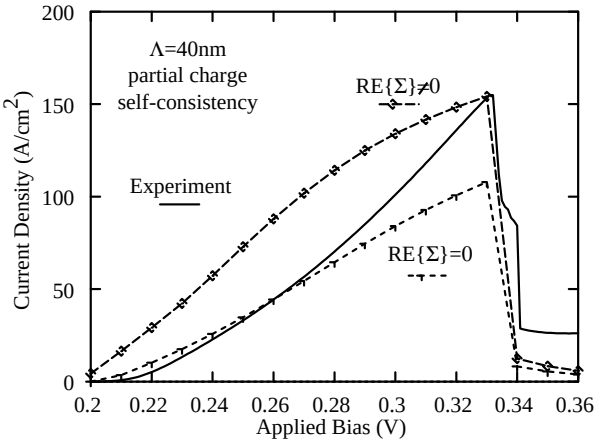

Figure 2. I–V characteristics for a single Λ = 40 nm comparing the effect of the inclusion and exclusion of the real part of the scattering self-energies explicitly. The potential is based on partial charge self-consistency. The I–V peak is significantly distorted if the real part of the scattering self-energies is included. Experimental data in the full line.

3. Full charge self-consistent simulations

The distortions in the shape and amplitude of the I–V characteristics indicate that the resonance spectrum in the RTD is significantly changed. This implies that the charge distribution in the device may be changed significantly as well. We now include the scattering-assisted charge in the charge self-consistent loop and again examine the effects of the exclusion and inclusion of the real part of the scattering self-energies.

If the real part of the scattering self-energies is excluded (see figure 3(*b*)), the peak amplitudes remain (see figure 1(*b*)) strongly reduced with increasing scattering strength. In addition, the I–V turn-offs are shifted to lower voltages.

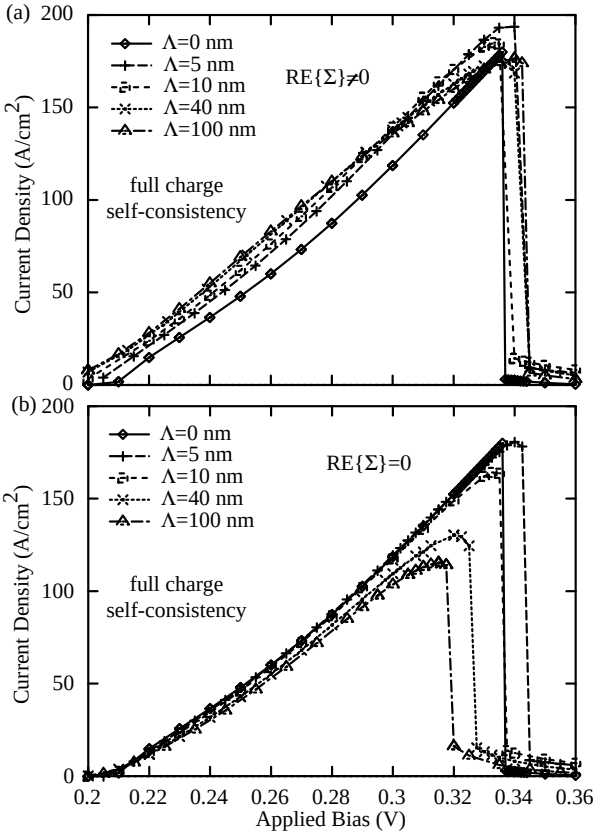

Figure 3. *I–V* characteristic for four different IR correlation lengths (Λ) computed on a full charge self-consistent potential including the effects of the scattering-assisted charge (*a*) including and (*b*) excluding the real part of the scattering self-energies.

If no approximations are made and the scattering-assisted charge and the real parts of the scattering self-energies are included (see figure 3(*a*)), the *I–V* curves are no longer distorted and they compare closely with the resonant current calculated with the coherent tunnelling model. Figure 4 compares the $\Lambda = 40$ nm curves from figure 3 with the experimental data.

4. The valley current

Finally, the effects of the real part of the self-energies on the RTD valley current are compared for various IR correlation lengths ($\Lambda = 5, 10, 40, 100$ nm) in the full charge self-consistent simulation. The coherent valley current ($\Lambda = 0$ nm) is for this device 2–3 orders of magnitude lower than the scattering-enhanced valley current and therefore not shown. In the valley current region, the current and the occupation of the well are small. Therefore, the effects of charging are expected to be small. We have indeed verified this and defer this discussion to a separate publication [14].

However, we have seen in section 3 that the real part of the scattering self-energies has a strong effect on the peak amplitude and peak voltage of the RTD. Figure 5 compares the valley current computed with and without the real part of the scattering self-energies. The simulations

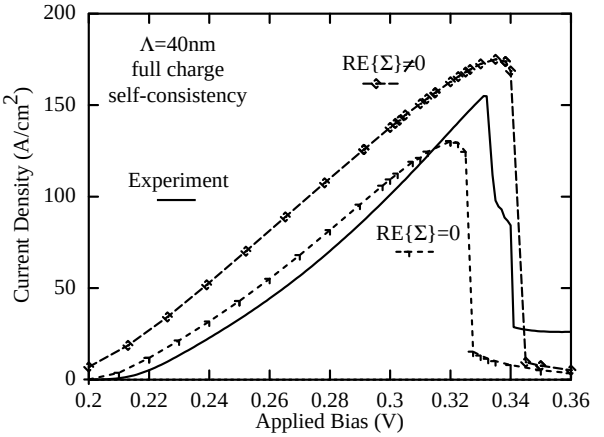

Figure 4. *I–V* characteristics for a single Λ = 40 nm comparing the effect of the inclusion or exclusion of the real part of the scattering self-energies. The potential is based on full charge self-consistency, which includes the effects of the scattering-assisted charge. The *I–V* peak is reduced and the peak voltage is shifted to lower values if the real part of the scattering self-energies is excluded from the simulation. Experimental data in the full line.

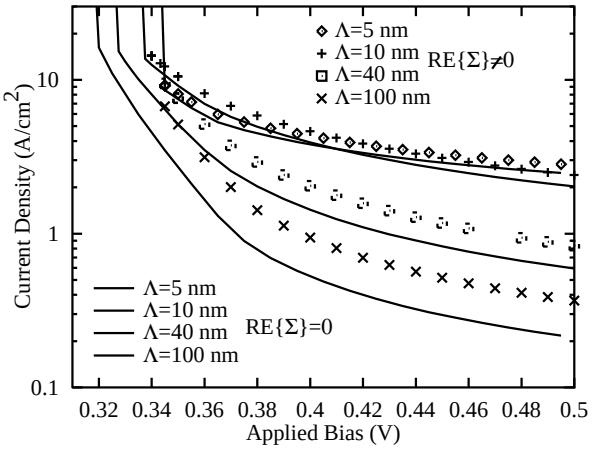

Figure 5. Valley current calculated in full charge self-consistency for four different IR correlation lengths (Λ) with and without the real parts of the scattering self-energies.

without the real part appear shifted to lower voltages from the corresponding simulations with the real part. This shift to lower voltages was already evident in figure 3(*b*). In this presentation we are not intending to simulate fully the valley current. It is shown in [6, 7] that the valley current can be properly modelled with the inclusion of polar optical phonon and IR scattering.

5. Summary

The effects of IR scattering have been computed in the self-consistent Born algorithm for various IR correlation lengths, charging models and self-energy approximations. For small average island sizes, $\Lambda \leq 5$ nm, the peak current is relatively unaffected by the approximation used. For larger average island sizes, a fully charge self-consistent

solution combined with both the real and the imaginary parts of the scattering self-energy are required for our device to reproduce the coherent tunnelling calculation of the resonant current. Any approximations lead to spurious distortion of the resonant current, while the off-resonant current is relatively unaffected.

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